

MgB₂C₂ Structure:

A2B2C_oC80_64_efg_efg_df-001

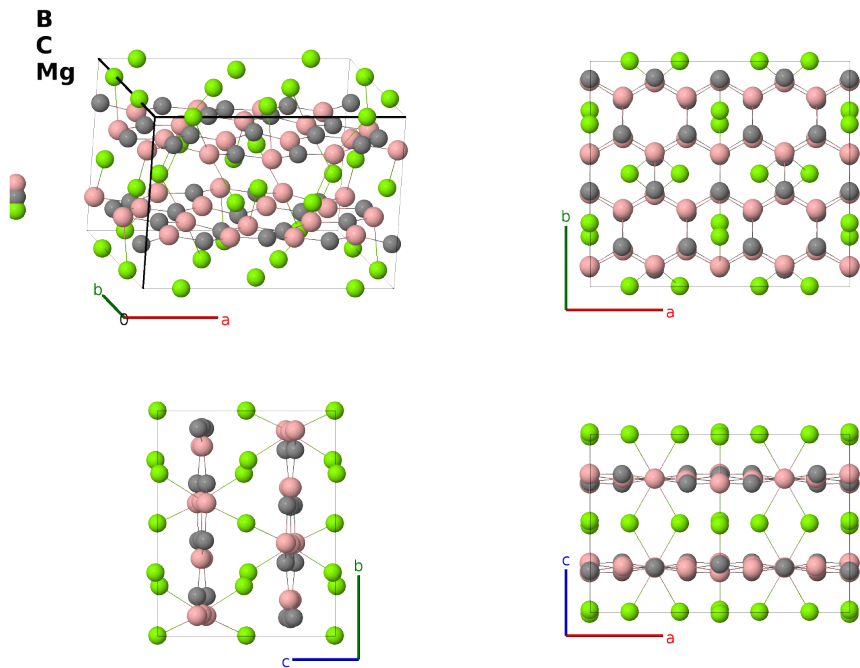
This structure previously used the label(s) **A2B2C_oC80_64_efg_efg_df**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/BJ3W>

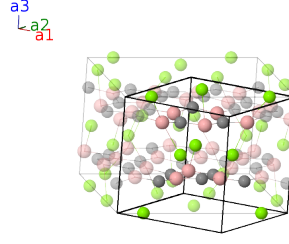
https://aflow.org/prototype-encyclopedia/A2B2C_oC80_64_efg_efg_df-001



Prototype	B ₂ C ₂ Mg
AFLOW prototype label	A2B2C_oC80_64_efg_efg_df-001
ICSD	79587
CCDC	1639833
Pearson symbol	oC80
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<pre>aflow --proto=A2B2C_oC80_64_efg_efg_df-001 --params=a,b/a,c/a,x₁,y₂,y₃,y₄,z₄,y₅,z₅,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈</pre>

Base-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 =$		$ax_1 \hat{\mathbf{x}}$	(8d)	Mg I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Mg I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 =$		$-ax_1 \hat{\mathbf{x}}$	(8d)	Mg I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 =$		$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Mg I
$\mathbf{B}_5$	$= -\left(y_2 - \frac{1}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$		$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	B I
$\mathbf{B}_6$	$= \left(y_2 + \frac{1}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$		$\frac{1}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	B I
$\mathbf{B}_7$	$= \left(y_2 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$		$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	B I
$\mathbf{B}_8$	$= -\left(y_2 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$		$\frac{3}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	B I
$\mathbf{B}_9$	$= -\left(y_3 - \frac{1}{4}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$		$\frac{1}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	C I
$\mathbf{B}_{10}$	$= \left(y_3 + \frac{1}{4}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$		$\frac{1}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	C I
$\mathbf{B}_{11}$	$= \left(y_3 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$		$\frac{3}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	C I
$\mathbf{B}_{12}$	$= -\left(y_3 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$		$\frac{3}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	C I
$\mathbf{B}_{13}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 =$		$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	B II
$\mathbf{B}_{14}$	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 =$		$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	B II
$\mathbf{B}_{15}$	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 =$		$\frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	B II
$\mathbf{B}_{16}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 =$		$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	B II
$\mathbf{B}_{17}$	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 =$		$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B}_{18}$	$= \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 =$		$\frac{1}{2}a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B}_{19}$	$= -\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 =$		$\frac{1}{2}a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B}_{20}$	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 =$		$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B}_{21}$	$= -y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 =$		$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8f)	Mg II

$$\begin{aligned}
\mathbf{B}_{22} &= \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2} \right) \hat{\mathbf{z}} &(8f) &\text{Mg II} \\
\mathbf{B}_{23} &= - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2} \right) \hat{\mathbf{z}} &(8f) &\text{Mg II} \\
\mathbf{B}_{24} &= y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(8f) &\text{Mg II} \\
\mathbf{B}_{25} &= \begin{pmatrix} x_7 - y_7 \\ z_7 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_7 + y_7 \\ z_7 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_7 - y_7 \\ z_7 \end{pmatrix} \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{26} &= \begin{pmatrix} -x_7 + y_7 + \frac{1}{2} \\ x_7 + y_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} -x_7 + y_7 + \frac{1}{2} \\ x_7 + y_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} -x_7 + y_7 + \frac{1}{2} \\ x_7 + y_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_7 - \frac{1}{2} \right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{27} &= \begin{pmatrix} -x_7 + y_7 - \frac{1}{2} \\ -x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_7 + y_7 - \frac{1}{2} \\ -x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} -x_7 + y_7 - \frac{1}{2} \\ -x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_7 - \frac{1}{2} \right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{28} &= \begin{pmatrix} x_7 + y_7 \\ z_7 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_7 - y_7 \\ z_7 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_7 + y_7 \\ z_7 \end{pmatrix} \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{29} &= - \begin{pmatrix} x_7 - y_7 \\ z_7 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_7 + y_7 \\ z_7 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_7 - y_7 \\ z_7 \end{pmatrix} \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{30} &= \begin{pmatrix} x_7 - y_7 + \frac{1}{2} \\ x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_7 - y_7 + \frac{1}{2} \\ x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_7 - y_7 + \frac{1}{2} \\ x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_7 + \frac{1}{2} \right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{31} &= \begin{pmatrix} x_7 + y_7 + \frac{1}{2} \\ x_7 - y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_7 + y_7 + \frac{1}{2} \\ x_7 - y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_7 + y_7 + \frac{1}{2} \\ x_7 - y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_7 + \frac{1}{2} \right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{32} &= - \begin{pmatrix} x_7 + y_7 \\ z_7 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_7 - y_7 \\ z_7 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_7 + y_7 \\ z_7 \end{pmatrix} \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(16g) &\text{B III} \\
\mathbf{B}_{33} &= \begin{pmatrix} x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(16g) &\text{C III} \\
\mathbf{B}_{34} &= \begin{pmatrix} -x_8 + y_8 + \frac{1}{2} \\ x_8 + y_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} -x_8 + y_8 + \frac{1}{2} \\ x_8 + y_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} -x_8 + y_8 + \frac{1}{2} \\ x_8 + y_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_8 - \frac{1}{2} \right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{C III} \\
\mathbf{B}_{35} &= \begin{pmatrix} -x_8 + y_8 - \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} -x_8 + y_8 - \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} -x_8 + y_8 - \frac{1}{2} \\ -x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \left(x_8 - \frac{1}{2} \right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{C III} \\
\mathbf{B}_{36} &= \begin{pmatrix} x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(16g) &\text{C III} \\
\mathbf{B}_{37} &= - \begin{pmatrix} x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(16g) &\text{C III} \\
\mathbf{B}_{38} &= \begin{pmatrix} x_8 - y_8 + \frac{1}{2} \\ x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 - y_8 + \frac{1}{2} \\ x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_8 - y_8 + \frac{1}{2} \\ x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_8 + \frac{1}{2} \right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{C III} \\
\mathbf{B}_{39} &= \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ x_8 - y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ x_8 - y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 + y_8 + \frac{1}{2} \\ x_8 - y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \left(x_8 + \frac{1}{2} \right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2} \right) \hat{\mathbf{z}} &(16g) &\text{C III} \\
\mathbf{B}_{40} &= - \begin{pmatrix} x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_8 - y_8 \\ z_8 \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 + y_8 \\ z_8 \end{pmatrix} \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(16g) &\text{C III}
\end{aligned}$$

References

- [1] M. Wörle and R. Nesper, *MgB₂C₂, a new graphite-related refractory compound*, J. Alloys Compd. **216**, 75–83 (1994), doi:10.1016/0925-8388(94)91045-6.

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